

# Discussion on Ohta et al., “Traveling bands in self-propelled soft particles”

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**Abstract.** A discussion on the contribution of Ohta and Yamanaka [1] in this special issue, supplemented by new agent-based simulations of band collisions within the standard Vicsek-model.

## 1 Motivation

In contribution [1] (see also [2]), the authors introduce a model of self-propelled deformable particles with a soft-core and alignment interactions. Performing agent-based numerical simulations, they study the formation of different kinds of traveling bands and, in particular, they investigate the behavior of these solitary bands in head-on collisions. This is an interesting study; it extends our own work on band collisions [3] in the simplistic Vicsek-model (VM) [4] to more realistic systems of particles with (soft) excluded volume interactions and non-spherical shape.

In the conclusion of contribution [1] the authors contrast their results with our previous results [3] and report opposite behavior. Specifically, they observe that bands of different size become of comparable size in subsequent collisions whereas we predicted that the initial height difference of the bands amplifies in collisions leading to the scenario of “larger eats smaller”.

In the first part of this comment, we would like to point out that the different behavior is not a contradiction because we believe the models used in Ref. [1] and previous papers [2,5,6] are in a different category than the regular Vicsek-model with polar alignment. In the second part, we would like to rule out possible errors on our side and report on corresponding agent-based simulations by the Vicsek-model. In Ref. [3] we showed quantitative agreement between kinetic theory and agent-based simulations for one single, stationary solitary wave in the limit of large mean-free path and studied head-on collisions by numerically integrating the kinetic equations. However, until now, we have never compared these collision studies to agent-based simulations. This missing link is now presented here. These new simulations confirm our previous observations: In the parameter region we explored, we never saw that the relative height difference between two waves of significantly different size decreases. Here, the height difference was always measured at sufficiently large separation of the two waves.

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## 2 Model analysis and comparison to Vicsek model

In this model [1,5], the shape of a particle with label  $i$  is phenomenologically described by means of a deformation tensor  $S_{\alpha\beta}^{(i)}$  that becomes relevant when particle-particle interactions occur. This tensor encodes the degree of deformation  $s^{(i)}$  and  $\mathbf{n}^{(i)}$ , the unit normal along the long axis of the deformed particle. The evolution equations for the velocities and deformation tensors, Eqs. (2)-(4) in [1], can be rewritten in terms of the particle speeds  $v^{(i)}$ , deformations  $s^{(i)}$ , flying direction  $\Phi^{(i)}$  (the angle between the particle velocity and the  $x$ -axis) and the angle  $\theta^{(i)}$  of the unit normal of the particle with respect to the  $x$ -axis as given in Eqs. (4)-(8) of Ref. [5].

Analysing the stationary states of these coupled equations for a single particle at the parameter values used in this contribution,  $a = 1$ ,  $b = 0.5$ ,  $\gamma_0 = \kappa = 1$ , one finds that (i) the particle undergoes stable ballistic motion (assuming zero noise  $\eta$ ) with constant speed  $v_0$  and elongates when flying; the larger  $v_0$  the more elongated it becomes, (ii), the flying direction is parallel/anti-parallel to  $\mathbf{n}^{(i)}$ , that is  $\phi^{(i)} = \theta^{(i)} \pm \pi$ , and the particle travels into the direction of its largest semi-axis. The force and noise terms are in the equation for the particle velocities. Thus, if a particle is slowed down by another one or by an obstacle,  $s^{(i)}$  decreases and the particle becomes more spherical. Depending on the impact parameter of such an interaction, both the particle orientation  $\theta^{(i)}$  and the flying direction  $\phi^{(i)}$  might change.

Thus, in the model of Ohta *et al.* the traveling state of a single particle is characterized by four degrees of freedom, that are nontrivially and nonlinearly coupled, whereas the VM has only one parameter per particle: the traveling direction.

Given the many couplings present in the model of Ohta *et al.*, the system has the potential to exhibit a much richer dynamics than simple Vicsek-models. Its particles might do funny things under stress, for example when they run into a wall, have a collision with an incoming dense front of particles and so on. While the authors wrote quite a number of papers on their model, [5,6,2], performed a linear stability analysis and studied the transition to rotational motion, we were not able to find publications that systematically study collisions of just two particles or the interaction of one particle with a wall as a function of impact angle and model parameters. This could be very helpful for understanding the solitary wave collisions on a microscopic level. For example, one could ask what the maximum shape change of a particle is, can it become strongly squeezed in a collision, e.g. changes from prolate to oblate shape with negative  $s^{(i)}$ , and then escapes sideways? Can it switch temporarily to rotational motion when hit by others? What are the relaxation times to recover from collision-induced deformation compared to the time interval until the next collision? Recently, it also has been pointed out that short-range repulsion can induce a density-dependent particle speed and this coupling between speed and density can lead to a zoology of complex patterns [12,13,14]. We think it would be worthwhile to discuss and compare the current model with respect to these developments.

Apart from the additional degrees of freedom, there is a more fundamental difference to the Vicsek-model (VM): the symmetry of the alignment interactions. Recent classifications of active matter [7,8,9] for self-propelled particles without volume exclusion distinguish between (A) nematic objects with nematic interactions, (B) polar particles with polar alignment and, (C) polar particles with nematic alignment. The VM is in class (B), the nematic VM of Ref. [10,11] is in category (C).

At first sight, the current model seems to be in class (C) since the alignment rule, Eq. (11) of [1], has nematic symmetry, i.e. stays invariant if the angles  $\theta$  of the involved particles are changed to  $\theta \pm \pi$ . However, if this were the whole truth, the observed polarly ordered moving bands in Fig. 6 would be in contradiction with the results for the nematic VM [11] where stationary bands do not move and only show

nematic order (see Fig. 2(c) of [11]). The patterns obtained by Ohta *et al.* are actually closer to the ones obtained for polar particles with polar alignment and a speed that is density dependent. Thus, if one accepts the simple classification of dry active matter into three classes, the current model of deformable particles looks like a mixed case of (B) and (C) for the following reasons:

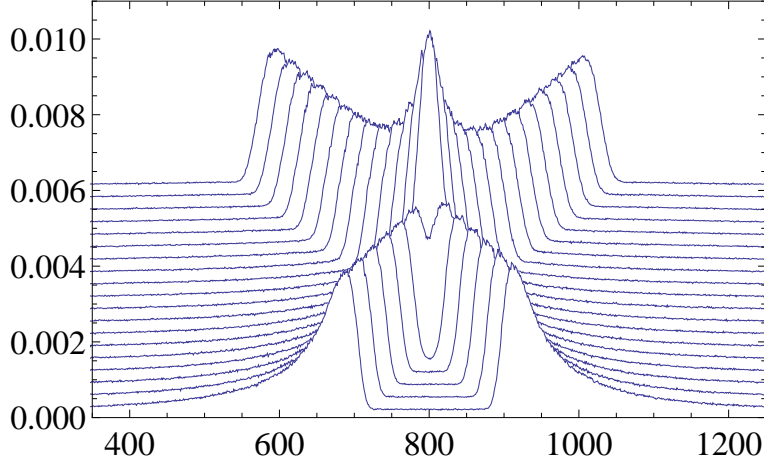
The collision rule of the nematic VM, Eq. (1) of [11], describes an idealized case of fast orientational relaxation. If one assumes the noise to be zero for the simplicity of this argument, perfect nematic alignment is already achieved in a single collision step. This does not have to be the case in a more realistic interaction. From Eqs. (4-8) of [5] one can read off finite relaxation times for the director relaxation, deformation and so on. If one assumes a grazing binary collision with  $\theta^{(i)} \approx -\theta^{(j)}$ , the relative particle speed is of order  $2v_0$  and the particles only have a contact time of order  $\tau_C \sim \sigma/v_0$  to attempt alignment. Here,  $\sigma$  is the effective radius of the deformable particle. If  $\tau_C$  is smaller than the relaxation time for alignment, the alignment will be incomplete. In contrast, if the particles have a parallel grazing collision, with  $\theta^{(i)} \approx \theta^{(j)}$  they will stay together much longer and achieve much better alignment. Thus, there is nematic alignment but it is biased towards parallel configurations. As a result, the interactions can be seen as a perfect nematic alignment plus a small polar alignment. We expect the relative importance of the polar component to be small for long rods, that is, particles with large aspect ratio.

Even though the particles in [1] are defined as points, the Gaussian soft-core potential, Eq. (9) together with the asymmetric factor  $Q_{ij}$  Eqs. (8), makes the particles interact like soft ellipsoids. Using Eqs. (7-11) of [1] with interaction strength  $Q = 50$  and the single-particle deformation  $s_0 = bv_0^2/\kappa = 0.4$ ,  $v_0^2 = \gamma_0/(1 + ab/(2\kappa)) = 0.8$ , it is possible to estimate the aspect ratio of these ellipsoids as between 2 and 3. This is quite small, the associated ellipsoidal shape of a particle is not too far from a sphere, and the polar component is likely to be nonnegligible. This could contribute to the existence of polar bands as opposed to the immobile nematic band of Ref. [11]. One could also speculate that a polar bias breaks the symmetry between parallel/antiparallel alignment and could be crucial even if very small. In any case, the qualitative difference between band collisions in the VM and the model of Ohta *et al.* raises interesting questions about universality in active matter.

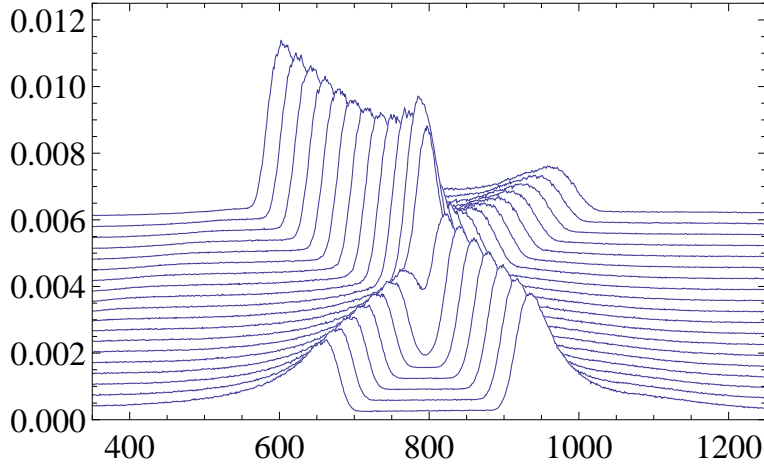
Another difference between Vicsek-like models such as the one studied in [10,11] and more realistic models such as the current model [1] is that in the former, particles can experience “frontal collisions” without much impact on their trajectories because of the absence of volume exclusion. Once there is at least a soft volume exclusion, nematic clusters where 50% of the particles come from the right and 50% from the left cannot exist. This would also support the occurrence of polar instead of purely nematic bands in Ref. [1].

In addition, the parameter  $\kappa = 1$  that controls the relaxation of a deformation is not large and, hence, the particles are presumably very soft. Because of the mixture of polar and nematic effects mentioned above and the softness of the particles, it is not totally surprising that the bands behave qualitatively different than in the regular Vicsek model. It would be interesting to isolate the possible reasons. For example, by increasing  $\kappa$ , ballistic motion should still be stable but the particles are less soft and one could check the influence of softness on solitary wave collisions.

The existence of a short range repulsion with effective radius  $\sigma = 1$  in the model of Ohta *et al.* [1] could be responsible for the flat region at the top of the density wave in Fig. 6 (b). For the VM, where particles have zero volume, the wave top is very spiky [3], see also Figs. 1 and 2.



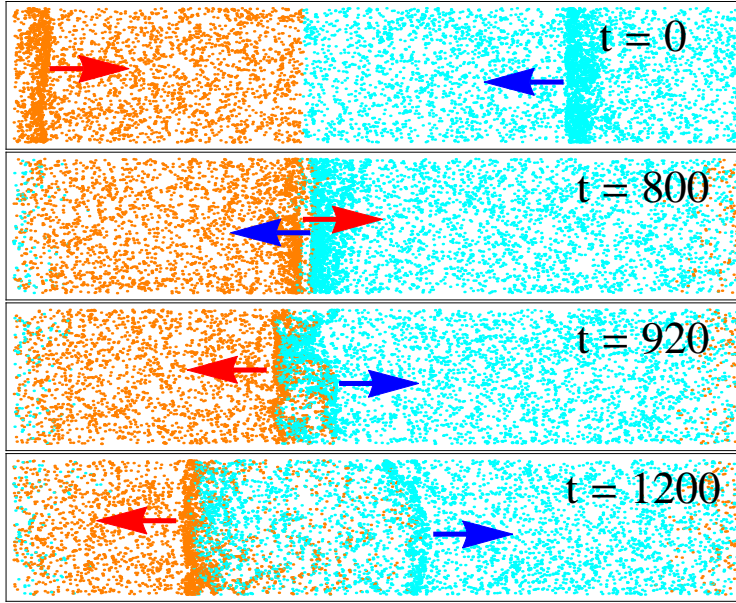
**Fig. 1.** Density snapshots for the head-on collision of two soliton-like waves obtained in agent-based simulations. The sequence starts with two well separated peaks close to the  $x$ -axis running towards collision with their steep fronts facing each other. At the latest time, the peaks are separated again after a successful “tunneling” through each other and now run towards the edges of the box. There is periodic boundary conditions in both  $x$  and  $y$  direction. Parameters (defined in Ref. [17]):  $M = \pi R^2 \rho_0 = 0.0393$ ,  $\tau v = 2$ , noise  $\eta = 0.46$ ,  $L_x = 1600$ ,  $L_y = 400$ , particle number  $N = 8000$ .



**Fig. 2.** Several snapshots of the density field of two colliding waves with significant height difference as a function of time for agent-based simulations of the VM. Parameters:  $M = 0.0393$ ,  $\tau v = 2$ ,  $\eta = 0.40$ ,  $L_x = 1800$ ,  $L_y = 400$ ,  $N = 9000$ .

### 3 Agent-based simulations

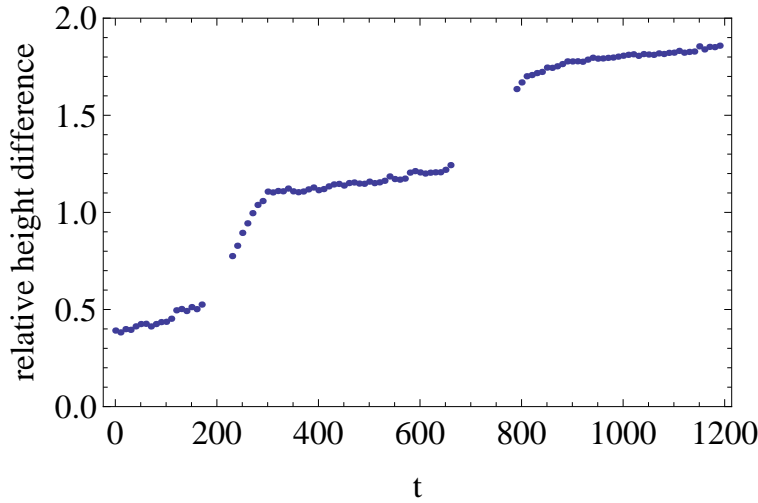
Here we repeat the “soliton collision test” as performed in [3] but now using agent-based simulations of the standard Vicsek-model instead of numerically solving the kinetic equation of the one-particle distribution function. We prepared stationary waves in two different systems with sizes  $L_x^{(1)}$  and  $L_x^{(2)}$ , particle numbers  $N_1$  and  $N_2$ , and ensured the waves run in opposite directions. After the waves became stationary, the two boxes were “glued” together leading to a longer system with  $L_x = L_x^{(1)} + L_x^{(2)}$ .



**Fig. 3.** Snapshots of two colliding waves at different for large density  $M = 0.7854$ . Only 20 % of all particles are shown. Parameters:  $\tau v = 0.5$ ,  $\eta = 1.6$ ,  $L_x = 1000$ ,  $L_y = 200$ ,  $N = 50000$ .

A series of snapshots of the time evolution of the density, averaged both over the  $y$ -direction and ensemble-averaged [16], is shown in Fig. 1 for very small initial height difference of the waves. At the earliest time, one sees two peaks running towards each other. Eventually, they start to overlap and form a large single peak. A while later, the two peaks reemerge with almost undisturbed shape like a conventional soliton. Watching the time evolution through repeated collisions reveals that if the waves have a tiny height difference initially, this difference is amplified in every encounter, as predicted by kinetic theory [3]. This increase of the height difference in a head-on collision becomes very clear in Fig. 2, where the two waves have quite different sizes already at the beginning. We found that this scenario is quite robust, even at larger densities, Fig. 3, and different noise  $\eta$ . However, at lower noise  $\eta$ , we observed a few cases, where both waves become smaller and slower in every collision, even though the relative height difference did not decrease. We interpret this behavior as the possibly discontinuous phase transition from an inhomogeneous ordered phase with solitons to the homogeneously ordered phase that is expected at small noise. Fig. 4 shows the relative height difference for parameters corresponding to Fig. 2. When the solitary waves collide, the height difference jumps up abruptly. No data points were taken right after the overlap of the wave peaks to allow the waves to “disentangle” and relax to two separate waves again.

By using large lateral lengths up to  $L_y = 2000$  (not shown) and aspect ratios  $L_y/L_x$  up to 1.5 we made sure to allow for the possible formation of waves going into the orthogonal  $y$ -direction after collision, something which is not possible by construction in the quasi-one dimensional runs of Ref. [3]. While we observed lateral fluctuations of the wave fronts, see Fig. 3 bottom, that are usually straight in systems with small  $L_y$ , we never saw waves that switch their propagation direction like Fig. 7(e) in Ohta *et al.* [1]. In large systems with  $L_y/L_x = 1.5$  we find that the time to recover to a straight wave front after collision is larger than the time  $L_x/v_w$  for the next collision that happens because of the periodic boundary condition over the



**Fig. 4.** Relative height difference  $2|h_1 - h_2|/(h_1 + h_2)$  versus time for the runs shown in Fig. 2. The maximum densities of the two waves are given by  $h_1$  and  $h_2$ , respectively.

shorter  $L_x$  direction. Here,  $v_w$  is the wave velocity. This velocity is larger than the speed of sound  $v_S$  in the disordered phase,  $v_S = v_0/\sqrt{2}$  [3]. As a consequence of the incomplete wave recovery, wave fronts show large fluctuations including partial break ups, until only one wave survives that does not undergo further collisions and thus has enough time to become straight. Even though we were not able to observe the scenarios reported by Ohta and Yamanaka, we cannot completely rule out this switch of wave direction as well as the possibility that bands of different size become of comparable size in subsequent collisions. This is because the relevant parameter space in density, noise and mean free path is quite large, and we mostly focused on parameters close to the ones used in [3].

To understand how solitons survive collisions, we “painted” the particles coming from the two different initial boxes in different colors, orange and cyan. For simplicity of the argument, we assume here that both waves have the same height (although this is *not* the case in Fig. 3, see [15]). At first sight, it seems as if both particle groups are reflected from the line where the wave fronts meet. However, looking very closely at the collision of the wave fronts in Fig. 3 and corresponding videos, we suggest a different mechanism: When the two wave fronts reach each other, small well aligned groups of particles penetrate the opposite front by a distance of the order of the mean free path  $\lambda = \tau v_0$ , where  $\tau$  is the time step of the Vicsek model and  $v_0$  is the particle speed. Since the density peak is very sharp, these groups are facing oppositely moving particles of the other color, that have a slightly smaller density and are thus slightly less aligned. Therefore, on average, these first penetrating groups manage to “overpower” the incoming particles in the tail of the opposite wave front and align them the other way [15]. Now, after these groups have been reinforced by particles of opposite color, they “sweep up” the rest of the incoming tail particles similar to a snowplow. This explains why the wave fronts in Fig. 3 after head-on collision seem to consist of two layers. The leading front contains now the newly piled up particles and in the tail one can see reminiscences of the original initiators of the change, which eventually fall behind and disappear from the main part of the wave. It would be interesting to see the difference between this mechanism and what is going on in the model of [1].



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15. Note, that the particle number per interaction circle of the VM is strongly fluctuating, in fact, even stronger than in an ideal gas, see [17]. Without fluctuations, the above argument could not explain how a small wave can survive confrontation with a much bigger wave.
16. In order to minimize artificial wave-broadening due to small speed differences of the waves, a specific type of ensemble average was used: The initial condition was fixed 1000 time steps before the two subsystems were “glued” together, and runs with different random number initializations were started from that position. We verified that snapshots from single realizations do not deviate too much from the ensemble average.
17. T. Ihle, Eur. Phys. J. Special Topics (2014), **this issue**.